TEMPEST:
Finite Volume Non-Linear Fokker-Planck Collision Operator

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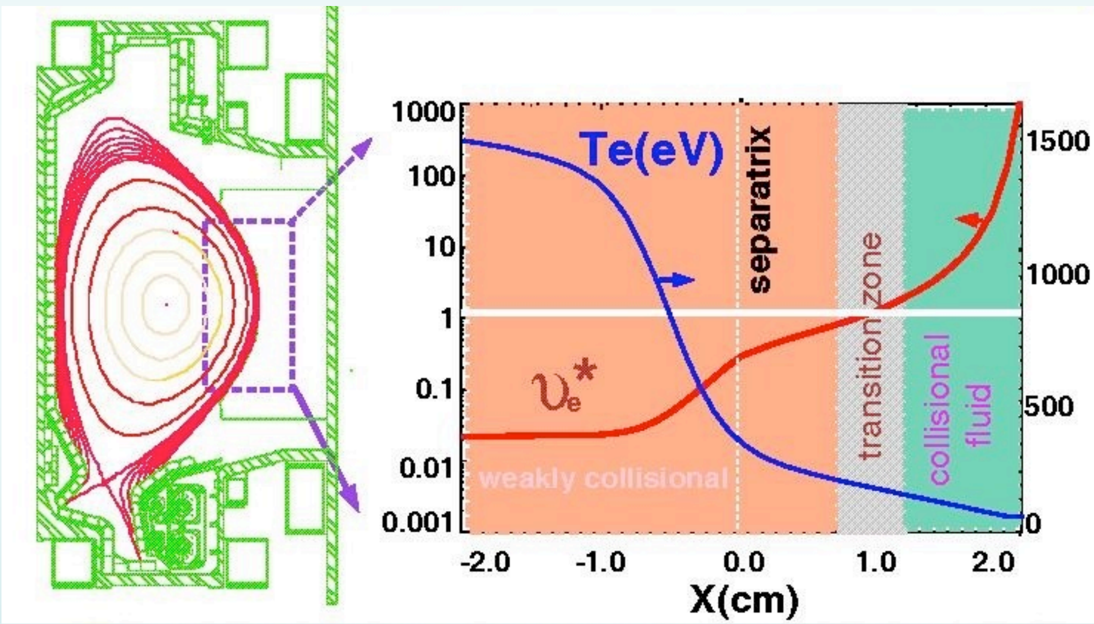
This work was performed for US DOE by LLNL under Contract W-7405-ENG-48.

Introduction

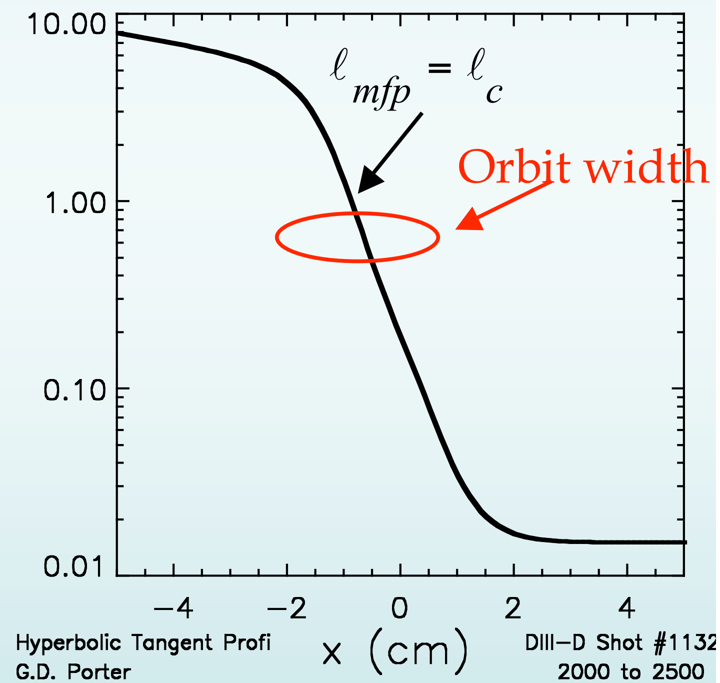
- Collision plays a crucial role in tokamak edge plasmas. Across a separatrix, the plasma collision frequency (ν^*) varies from <0.1 in the core (weakly collisional regime) to >10 in the edge (collisional fluid regime). At a H-mode pedestal, the ratio between particle mean free path and connection length is around unity.

Collision frequency ν^* across separatrix



DIII-D Edge Barrier

$\ell^{(e)}_{mfp}/\ell_c[x]$



- Edge kinetic simulations must be able to capture the collisional effects accurately and bridge the different collisional regimes.

TEMPEST

- TEMPEST is a 5 dimensional (3D+2V) gyrokinetic continuum code, currently being developed at LLNL, for studying the boundary plasma over a region extending from inside the H-mode pedestal across the separatrix to the divertor plates (find more details in the previous and next posters).
- TEMPEST solves gyro-kinetic equations for full distribution function F, and uses gyro-kinetic Poisson equation for self-consistent electric potential. The usual radial, poloidal and toroidal coordinates are (ψ,θ, ζ). In velocity space, the so-called the constants-of-motion coordinates are chosen, namely, energy (E) and magnetic moment μ. So $F = F(\psi,\theta, \zeta, E, \mu)$.
- In the collisionless limit, E and μ remain constant along particle orbits. The choice of (E, μ) thus enables an accurate and efficient algorithm for spatial advections, e.g. parallel streaming and radial drift, because it automatically avoids numerical diffusion in velocity space.
- For collisional cases, a Fokker-Planck collision (FPC) operator is needed.
- What is the velocity coordinates used in FPC ?

FPC in (V-θ) coordinates

- Collisions are ubiquitous, and FPC is widely used in many fields of plasma physics. Most of the existing FPCs, however, aimed at simulating spatially homogeneous plasmas, e.g.[1]. Therefore, a spherical coodinates (v, θ, ϕ), with assumed azimuthal symmetry, is used following Rosenbluth et al (1957).

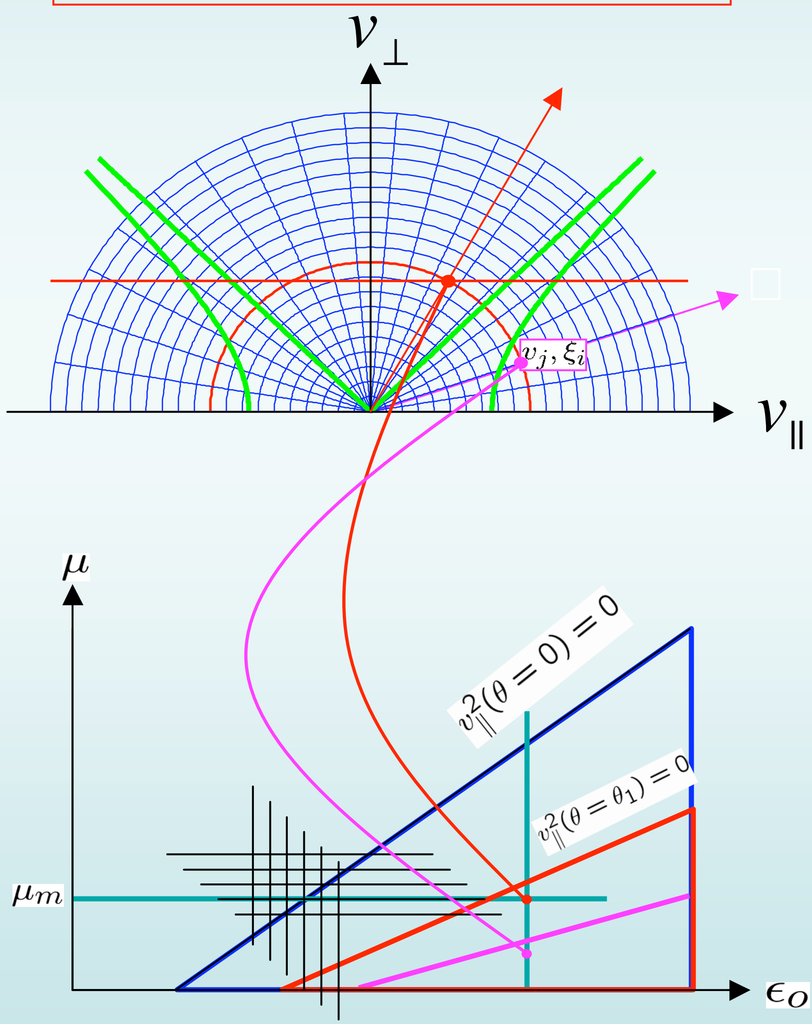
$$\frac{\partial F_\alpha}{\partial t} = \sum_\beta C_{\alpha\beta}(F_\alpha, F_\beta) \qquad \text{with} \quad F_\alpha = F_\alpha(v, \theta, t).$$

- With Legendre polynomial expansion in pitch angle (cosθ) for F and the so called Rosenbluth potentials, $C_{\alpha\beta}$ can be obtained by solving a system of second order ODEs. The solution is fast and easy.
- The development of fully nonlinear FPC in (V-θ) coordinates started around mid 80's, and it has been successfully applied in studying mirror machine confinement, RF heating, neutral beam injection, and so on [1].
- No need to reinvent the wheel. Why not just use the existing one ?

[1] J. Killeen, G.D. Kerbel, M.G. McCoy, A.A.Mirin,, Computational methods for kinetic models of magnetically confined plasmas. Springer Series in Compuational Physics.(1986).

First Attempt: interpolation

$$\frac{\partial F_\alpha}{\partial t} = \sum_\beta C_{\alpha\beta}(F_\alpha, F_\beta)$$



Approach:

1) Interpolating F from (E, μ) to a (v, θ) grid.
2) Compute Rosenbluth potentials and the diffusion coefficients.
3) Compute Cαβ(F,F) itself in (v, θ).
4) Interpolating Cαβ(F,F) back to (E, μ) grid

But this proves to be problematic:

1) Difficult to do accurate interpolation between the two meshes shown here, particularly for coarse grids.
2) Despite the fact that FPC in (v, θ) space conserves the number of particles, the particle conservation is lost during the interpolation,.
3) For energy and momentum, the conservation property are worse .

FPC in (E-μ) coordinate

- **Goal: improve conservation properties of FPC in (E, μ)**
  - –Interpolate only the diffusion *coefficients* (slow varying) from (v,θ).
  - –But do conservative flux difference in (E,μ) space directly with finite volume approach.
  - –Requires treatment of *cut cells* at turning point boundary.

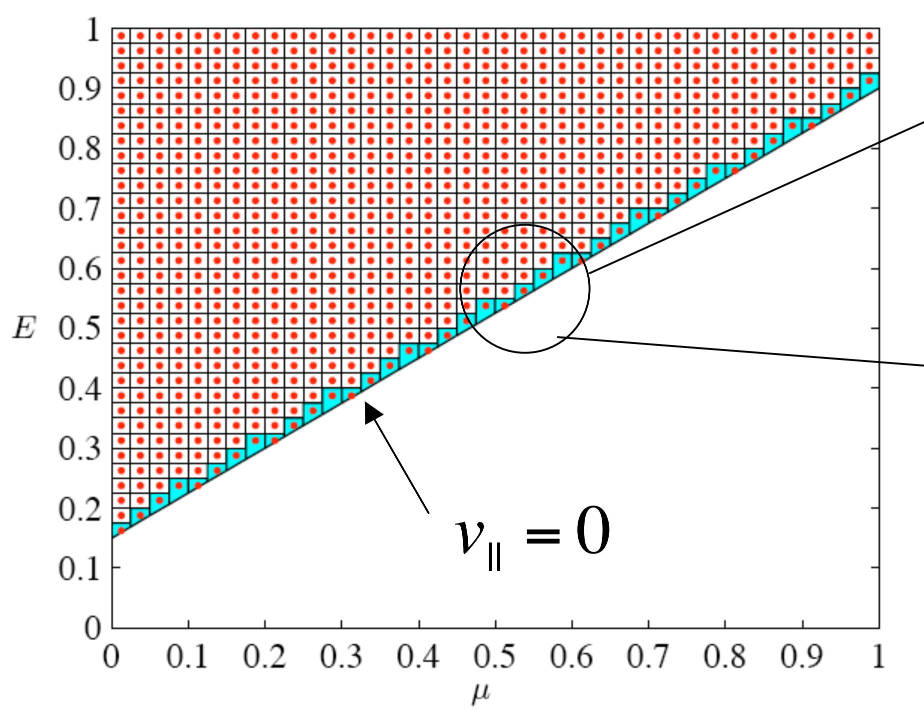
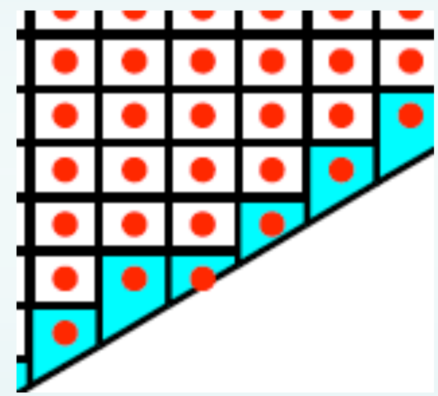


Figure 1: Velocity space in $E - \mu$ coordinates.



cut cells, cell -merging to avoid small cell problem!

Finite volume is inherently Conservative!

$V_{||}$-μ coordinates

- For numerical implementation, we further transform (analytically) the energy coordinate E into parallel velocity via $v_{\|} = \sqrt{2(E - \mu B - Z\phi)/m}$ so that for each cell in (E, μ) space, there are two corresponding cells in $v_{||}$ -μ space (for $v_{||} > 0$ and $v_{||} < 0$).

Advantages :

1. $v_{||}$ and μ are essential quantities for gyro-kinetic description.
2. $v_{||}$ -μ has a constant Jacobian.
3. avoid branch-cut problem at $v_{||}$ = o boundary when E is used.
4. no numerical interpolation is needed.

Transformed mesh from the previous page

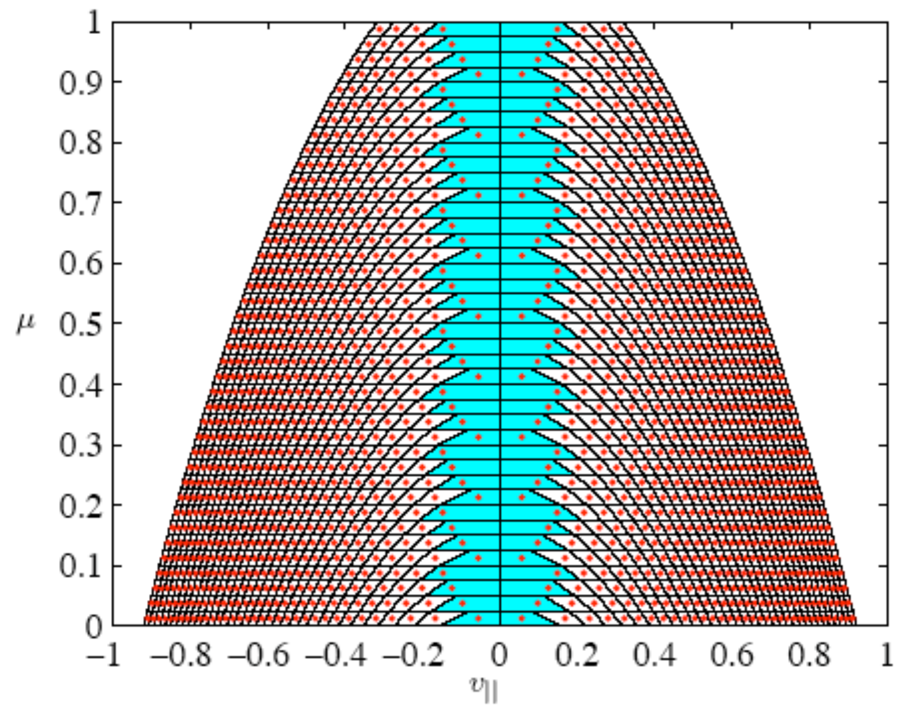


Figure 2: Velocity space in $v_{||} - \mu$ coordinates.

Nonlinear Formulation

Ignoring the gyro-phase, the divergence form of FPC in $v_{||}$ and μ is

$$C(f_\alpha) = -\frac{\partial S_x^{\alpha/\beta}}{\partial v_x} - \frac{\partial S_y^{\alpha/\beta}}{\partial v_y} - \frac{\partial S_z^{\alpha/\beta}}{\partial v_z} = \frac{\partial F_{v_{||}}}{\partial v_{||}} + \frac{\partial F_\mu}{\partial \mu} \qquad (1)$$

Where the fluxes are

$$\begin{aligned} F_{v_{||}} &= D_v f_\alpha + D_{vv}\frac{\partial f_\alpha}{\partial v_{||}} + D_{v\mu}\frac{\partial f_\alpha}{\partial \mu} \\ F_\mu &= D_\mu f_\alpha + D_{\mu v}\frac{\partial f_\alpha}{\partial v_{||}} + D_{\mu\mu}\frac{\partial f_\alpha}{\partial \mu} \end{aligned} \qquad (2)$$

and the diffusion coefficients are given by

$$\begin{aligned} D_v &= n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha}{\ } \frac{\partial h^\beta}{\partial} \\ D_{vv} &= -n_\beta \Lambda^{\alpha/\beta} \frac{\partial^2 g^\beta}{\partial v_{||}^2} \\ D_{v\mu} &= -2\, n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha}{B} \mu \frac{\partial^2 g^\beta}{\partial v_{||} \partial \mu} \end{aligned}$$

$$\begin{aligned} D_\mu &= 2 n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha^2}{B m_\beta} \mu \frac{\partial h^\beta}{\partial \mu} \\ D_{\mu v} &= -2 n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha}{B} \mu \frac{\partial^2 g^\beta}{\partial v_{||} \partial \mu} \\ D_{\mu\mu} &= -2 n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha^2}{B^2} \mu \left(2\mu \frac{\partial^2 g^\beta}{\partial \mu^2} + \frac{\partial g^\beta}{\partial \mu}\right) \end{aligned} \qquad (3)$$

The Trubnikov-Rosenbluth potentials (g, h) satisfy:

$$\begin{aligned} \frac{\partial^2 g^\beta}{\partial v_{||}^2} + \frac{m_\alpha}{B}\frac{\partial}{\partial \mu}\left(2\mu \frac{\partial g^\beta}{\partial \mu}\right) &= h^\beta \\ \frac{\partial^2 h^\beta}{\partial v_{||}^2} + \frac{m_\alpha}{B}\frac{\partial}{\partial \mu}\left(2\mu \frac{\partial h^\beta}{\partial \mu}\right) &= f_\beta . \end{aligned} \qquad (4)$$

Linearization of FP

If the collisions between the test particles and the background plasma is more important than the collisions among the test particle themselves, the full FPC can be linearized, as if the distribution function for the field particles is known, and often times, assumed to be Maxwellian. In such cases, the equation (3) becomes:

$$
\begin{aligned}
\tilde{D}_v &= n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha}{m_\beta} \frac{v_{||}}{v} \frac{dh^\beta}{dv} \\
\tilde{D}_{vv} &= -n_\beta \Lambda^{\alpha/\beta} \left(\frac{2\mu B}{m_\alpha v^3} \frac{dg^\beta}{dv} + \frac{v_{||}^2}{v^2} \frac{d^2 g^\beta}{dv^2} \right) \\
\tilde{D}_{v\mu} &= 2\, n_\beta \Lambda^{\alpha/\beta} \left(\frac{\mu v_{||}}{v^3} \frac{dg^\beta}{dv} - \frac{\mu v_{||}}{v^2} \frac{d^2 g^\beta}{dv^2} \right) \\
\tilde{D}_\mu &= 2 n_\beta \Lambda^{\alpha/\beta} \frac{m_\alpha \mu}{m_\beta v} \frac{dh^\beta}{dv} \\
\tilde{D}_{\mu v} &= 2\, n_\beta \Lambda^{\alpha/\beta} \left(\frac{\mu v_{||}}{v^3} \frac{dg^\beta}{dv} - \frac{\mu v_{||}}{v^2} \frac{d^2 g^\beta}{dv^2} \right) \\
\tilde{D}_{\mu\mu} &= 2 n_\beta \Lambda^{\alpha/\beta} \left[\left(\frac{2\mu^2}{v^3} - \frac{m_\alpha \mu}{vB} \right) \frac{dg^\beta}{dv} - \frac{2\mu^2}{v^2} \frac{d^2 g^\beta}{dv^2} \right].
\end{aligned}
$$

and the equation (4) can be solved as :

$$
\begin{aligned}
\frac{dh^\beta}{dv} &= \frac{1}{4\pi v^2} H\left(v\sqrt{\frac{m_\beta}{2T_\beta}}\right) \\
\frac{dg^\beta}{dv} &= \frac{T_\beta}{8\pi m_\beta v^2} H\left(v\sqrt{\frac{m_\beta}{2T_\beta}}\right) - \frac{1}{8\pi} G\left(v\sqrt{\frac{m_\beta}{2T_\beta}}\right) \\
\frac{d^2 g^\beta}{dv^2} &= -\frac{T_\beta}{4\pi m_\beta v^3} H\left(v\sqrt{\frac{m_\beta}{2T_\beta}}\right)
\end{aligned}
$$

Results presented in this poster are based on linear FPC calculations.

Non-Linear Coefficients

New Approach:

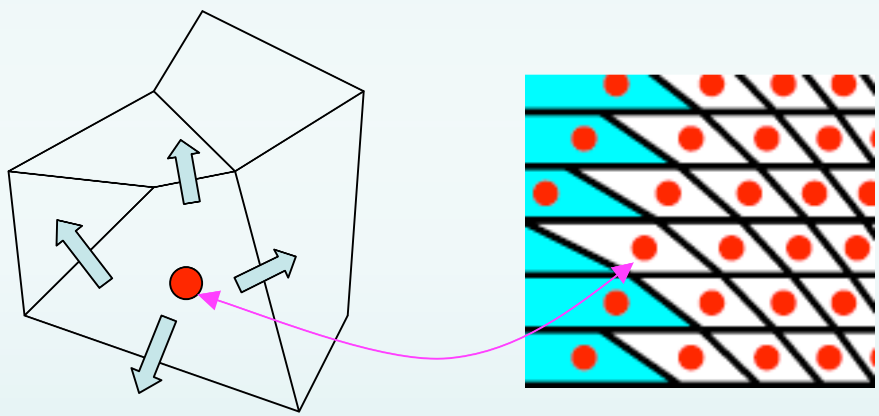
1) Interpolate F from (E,μ) to a (v,θ) grid using 4th order reconstruction technique
2) Compute Rosenbluth potentials and diffusion coefficients in (v, θ)
3) Interpolate NonLinear coefficients back to (v||, μ) grid
4) Compute conservative difference operator using coefficients for (v||, μ) reconstructed fluxes

Finite volume schem

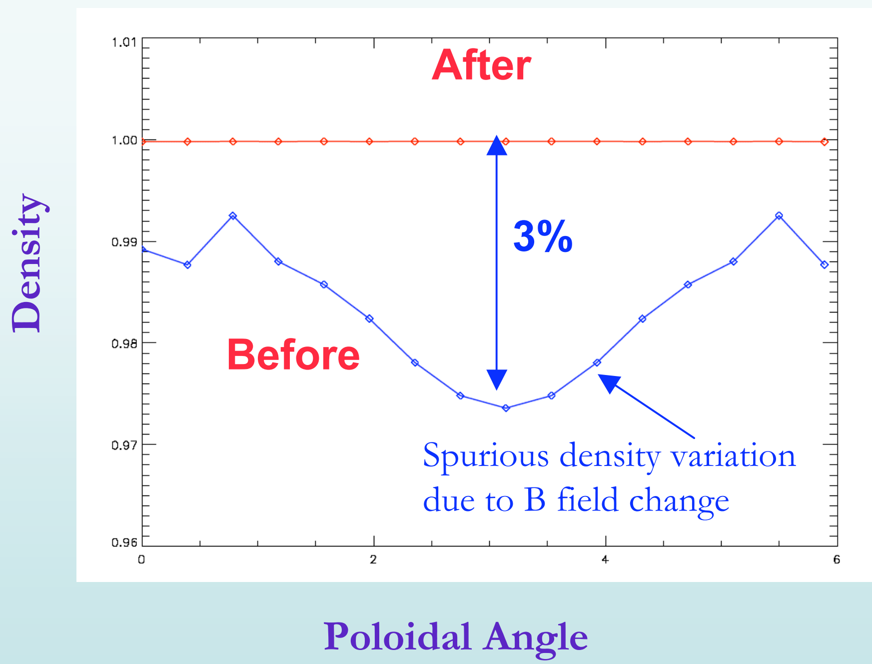
Unlike finite difference method, which uses point-wise function values, finite volume scheme solves the cell-integrated equation.

$$\frac{\partial f}{\partial t} + \nabla \cdot F(f) = 0 \qquad \Rightarrow \qquad \frac{\partial \bar{f}}{\partial t} = -\oiint_{cell} F \cdot dS$$

and the quantity that is being updated is the cell-averaged function value $\bar{f}$



An example: improvement made by cutting cells and finite volume approach for density moment



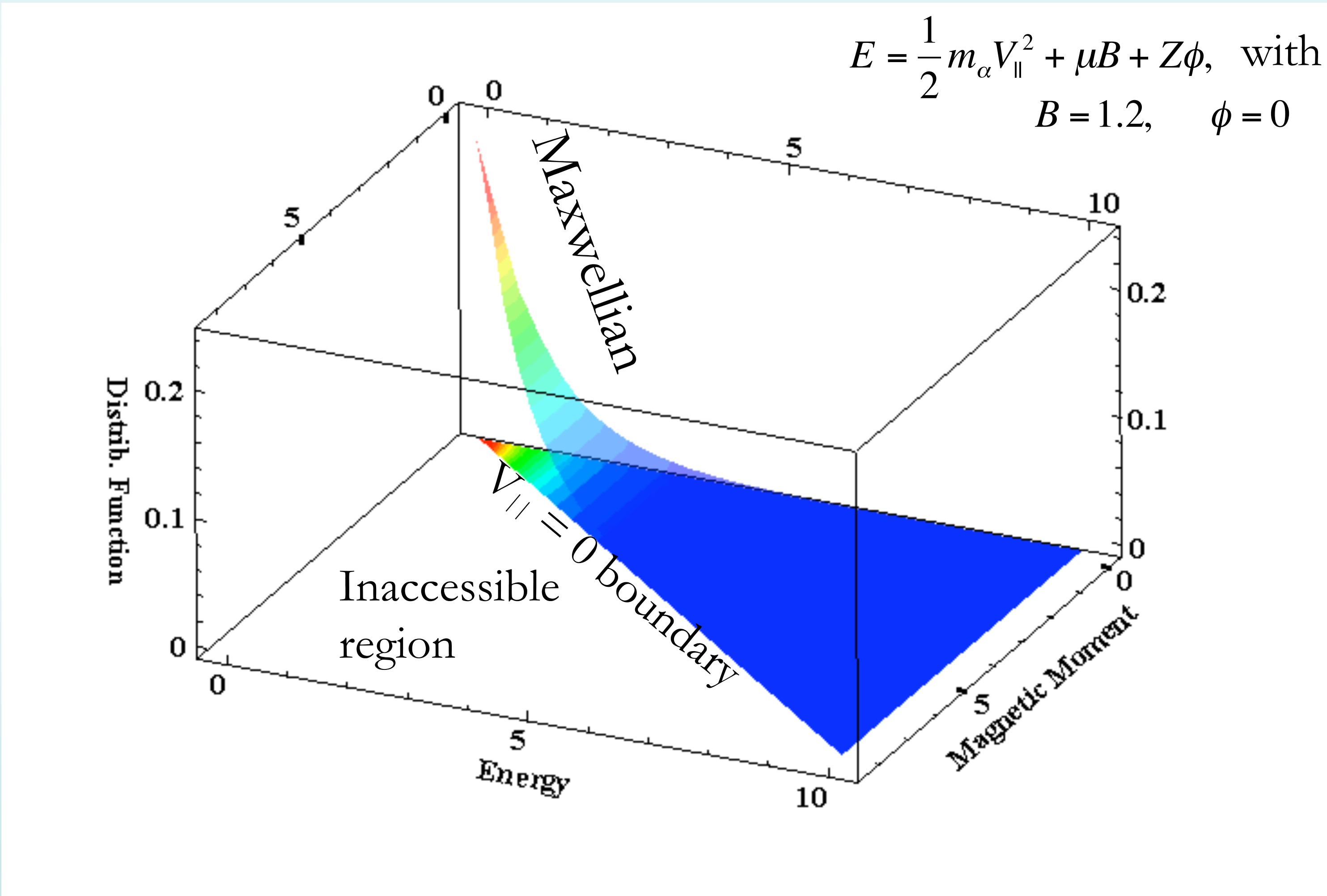
A reconstruction scheme is needed for getting point-wise values for computing edge fluxes.

By construction, finite volume scheme conserves overall particle density.

Initial conditio

- A Maxwellian distribution function with unit mean temperature (Tα=1) i (E, μ) space used as an initial condition for linear FPC calculation:

$$\boxed{\frac{\partial F_\alpha}{\partial t} = C(F_\alpha, F_\beta)}$$ α test particle, β field particle



Thermal Equilibration

- Time history of total energy for test particles during thermal equilibration

Runing parameters:

$$m_\alpha = m_\beta = 2m_p$$

$$Z_\alpha = Z_\beta = 1$$

$$T_\alpha(t=0) = 1(kev);$$

$$T_\beta = 1.5(kev) \quad (heating)$$

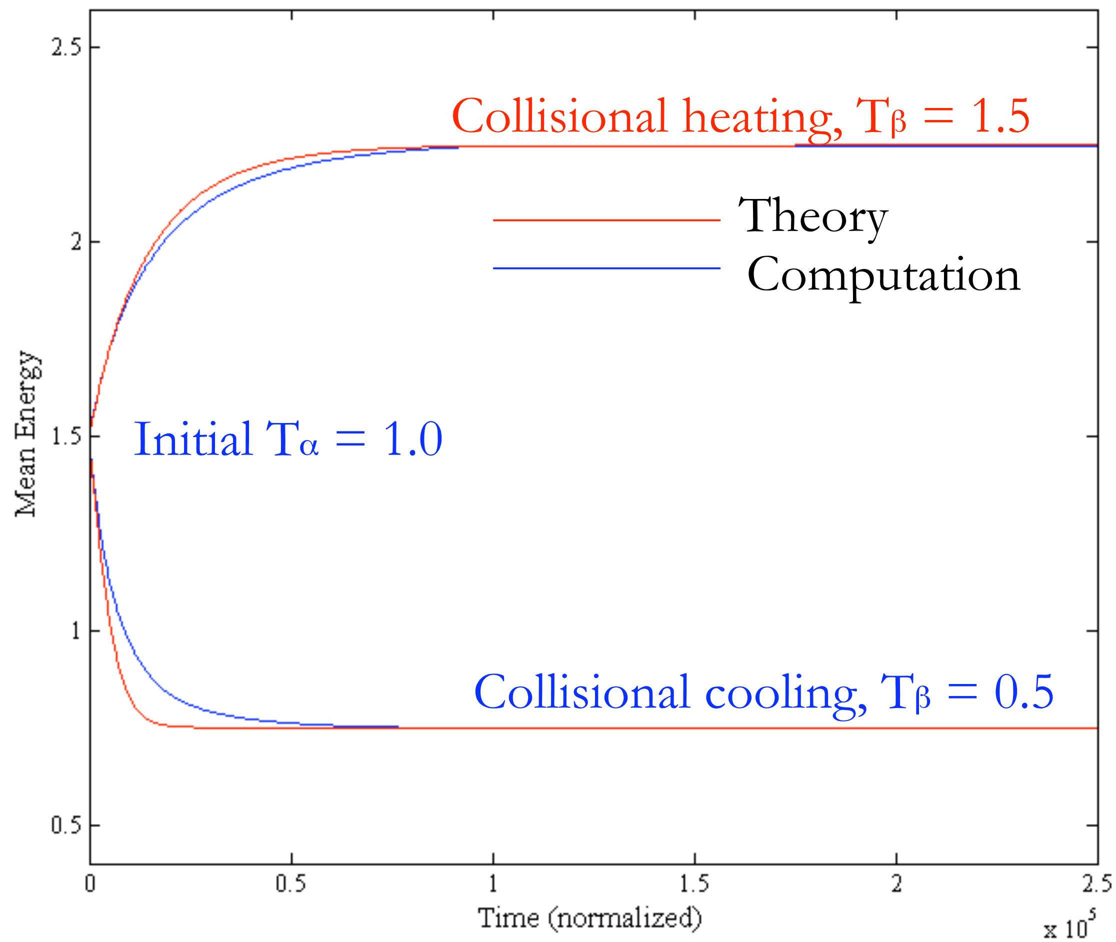
$$T_\beta = 0.5(kev) \quad (cooling)$$

$$\lambda = 21$$

$$n_\beta = 10^{15}(cm^{-3})$$

Total # of cells
in (E, μ) space

462



Relaxation Tim

- The initial rate of energy change in thermal equilibration is described by relaxation time (Spitzer(1940)).

$$\frac{dT_\alpha}{dt} = \frac{T_\beta - T_\alpha}{\tau_T^{\alpha/\beta}}$$

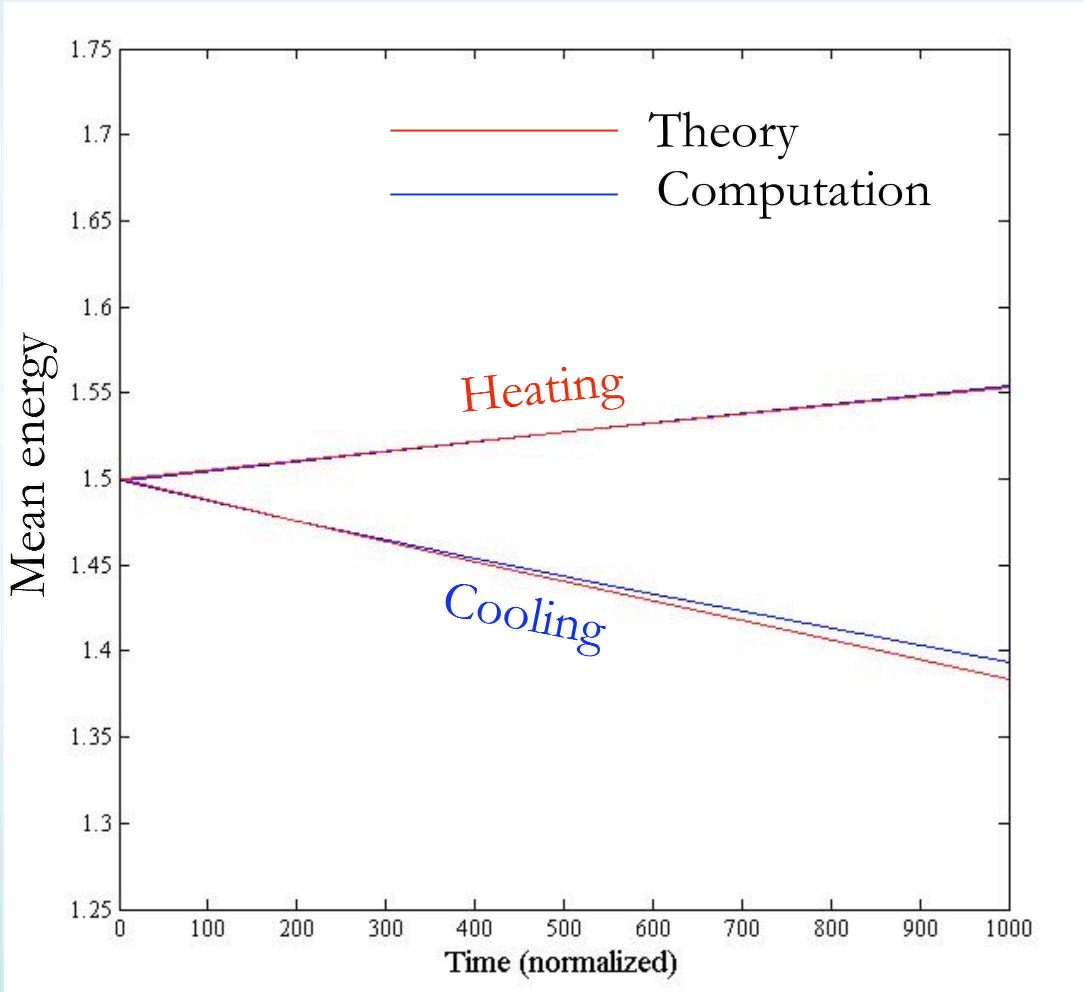
where

$$\tau_T^{\alpha/\beta} = \frac{3\sqrt{\pi}}{8}\tau_1^{\alpha/\beta}\left(T_\alpha + \frac{m_\alpha}{m_\beta}T_\beta\right)$$

and

$$\tau_1^{\alpha/\beta}(x) = \frac{\sqrt{m_\alpha}}{\pi\sqrt{2}e_\alpha^2 e_\beta^2}\frac{x^{3/2}}{\lambda n_\beta}$$

Theory assumes both distribution functions are Maxwellians.

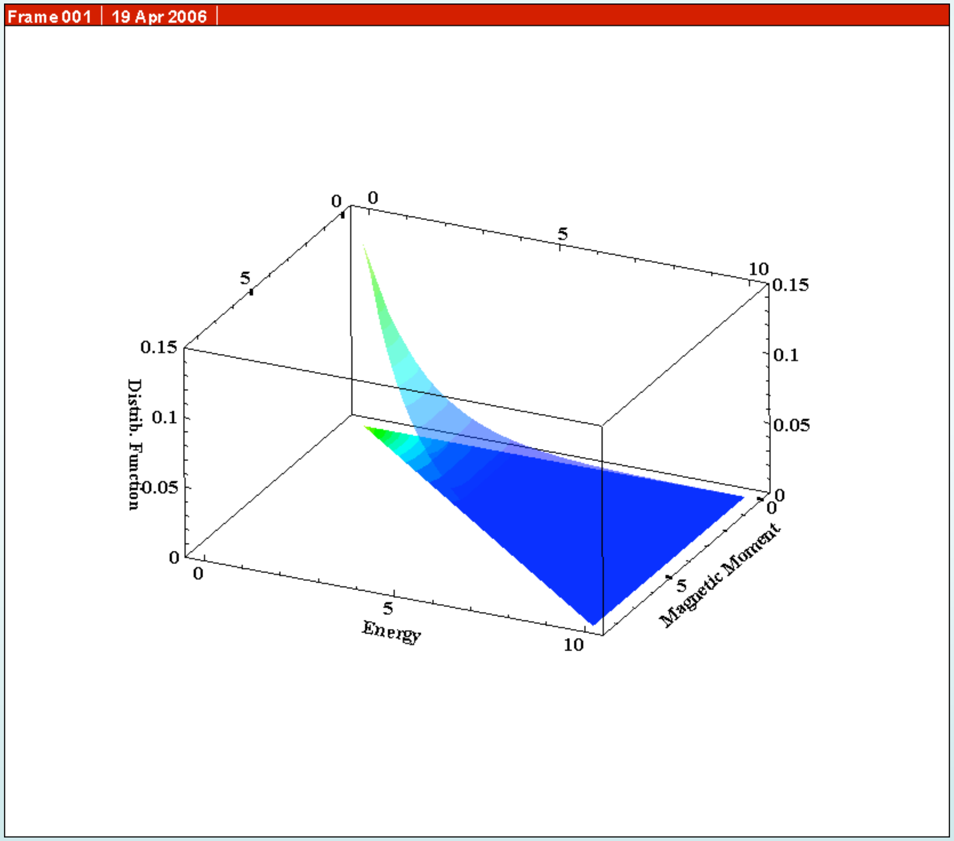


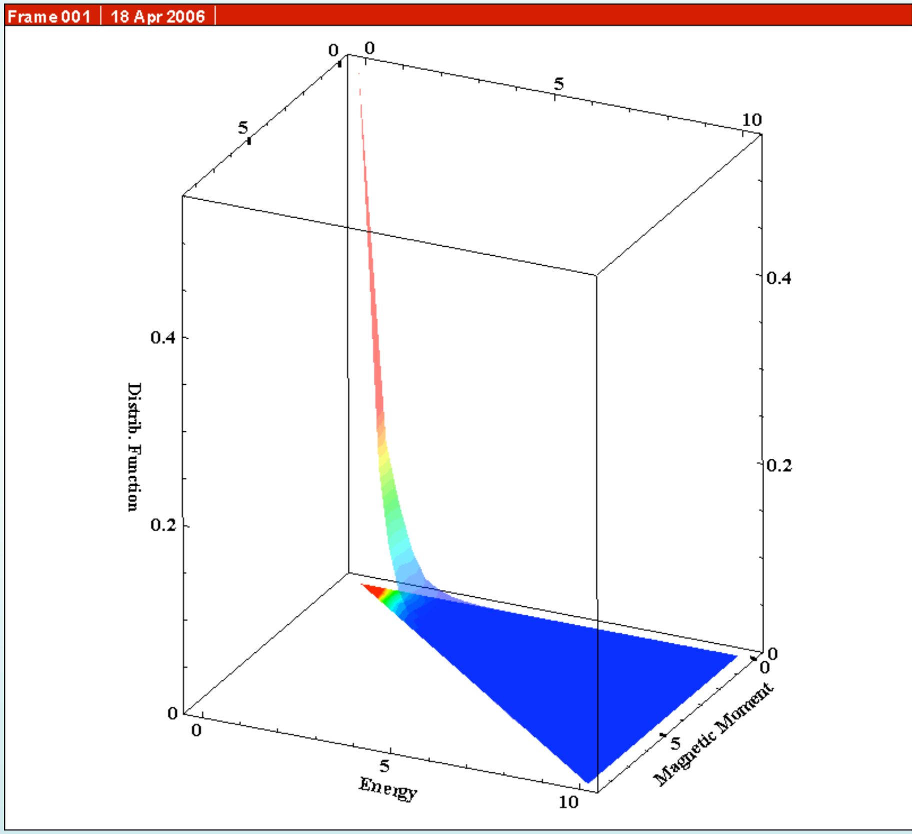
Distribution functions

- The final distribution functions for the test particles after thermal equilibration is reached.

Heating, Tα = 1.5 @ t = t_∞

Cooling, Tα = 0.5 @ t = t_∞

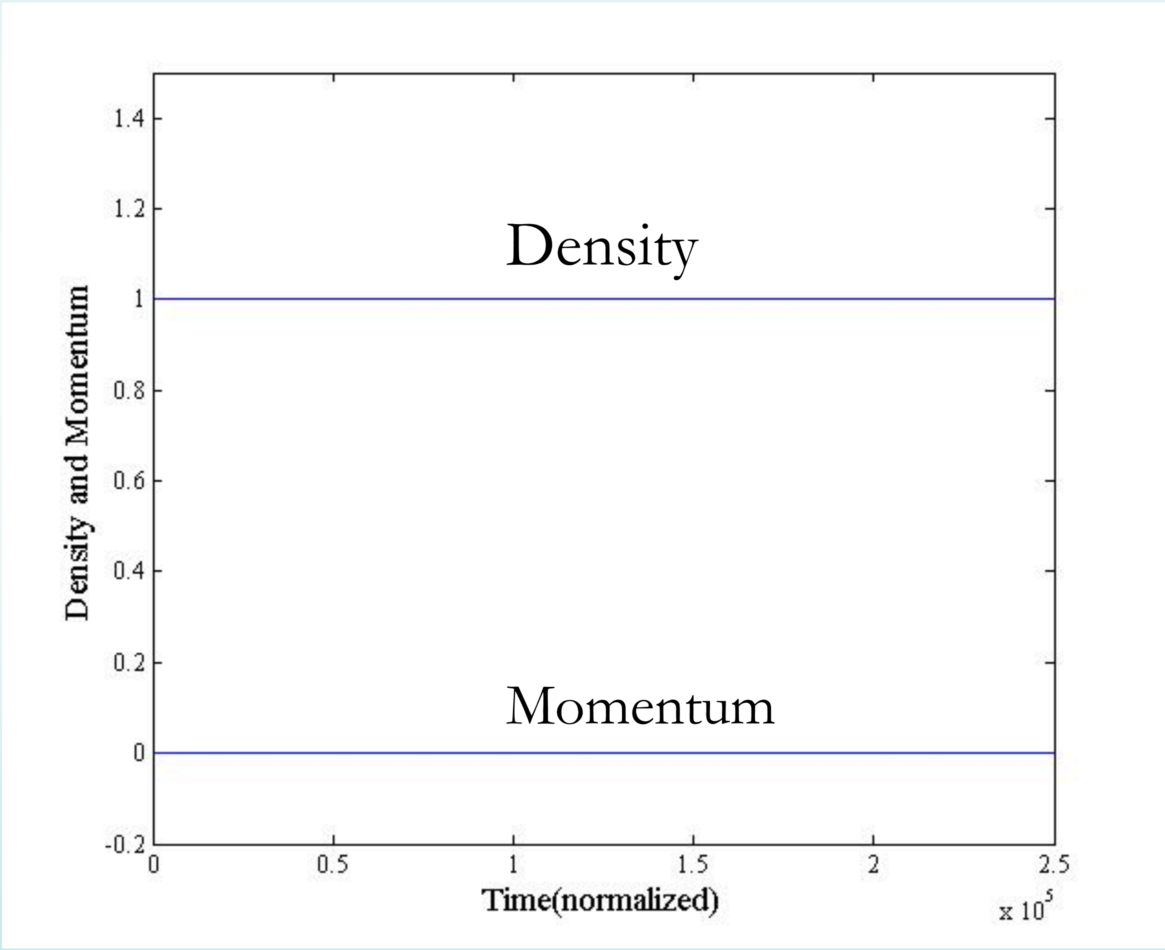




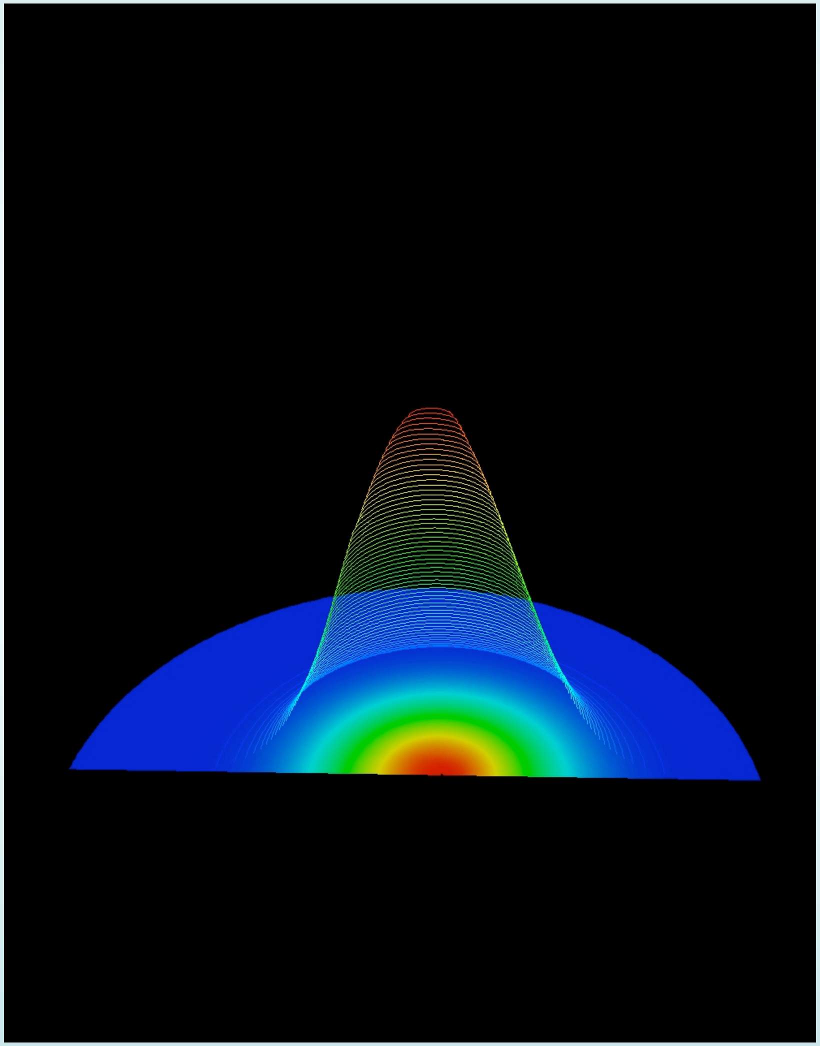
- Compare the initial distribution on page 11.

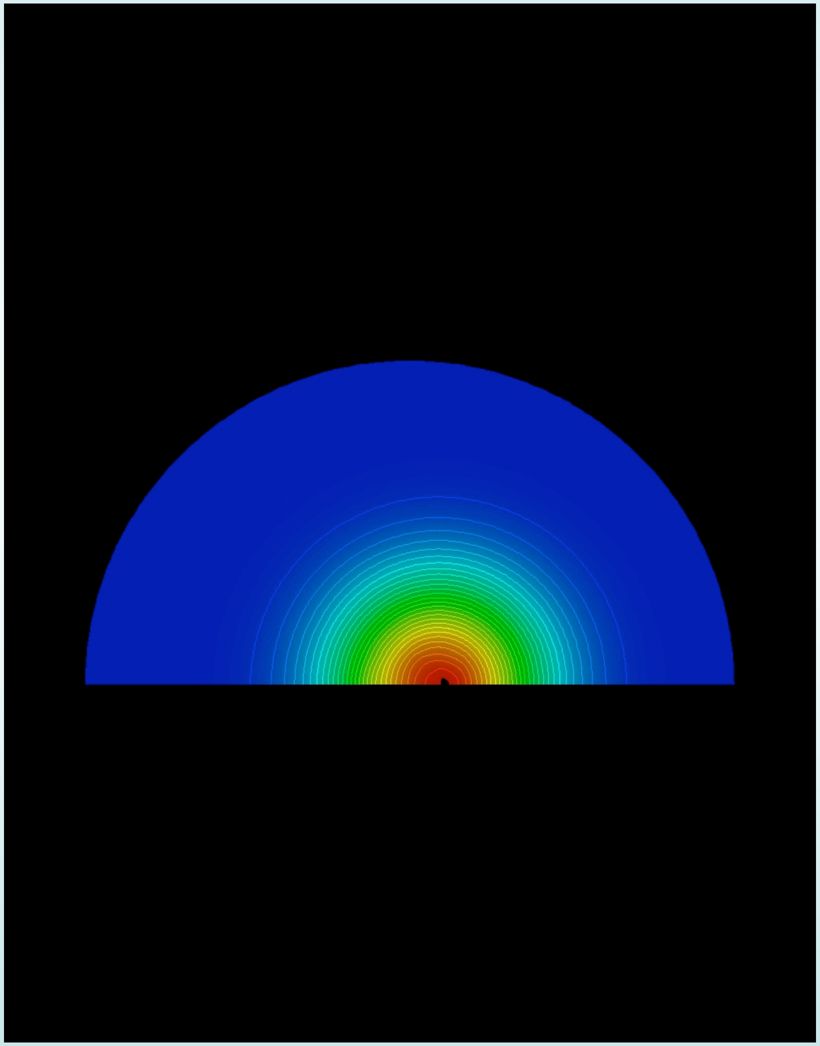
Density and Momentun

- During the thermal equilibration, the particle density is exactly conserved
- The momentum remains to be zero (initial value) throughout.



Drifting Maxwellian Test
Non-Linear Self Collision Annihilation

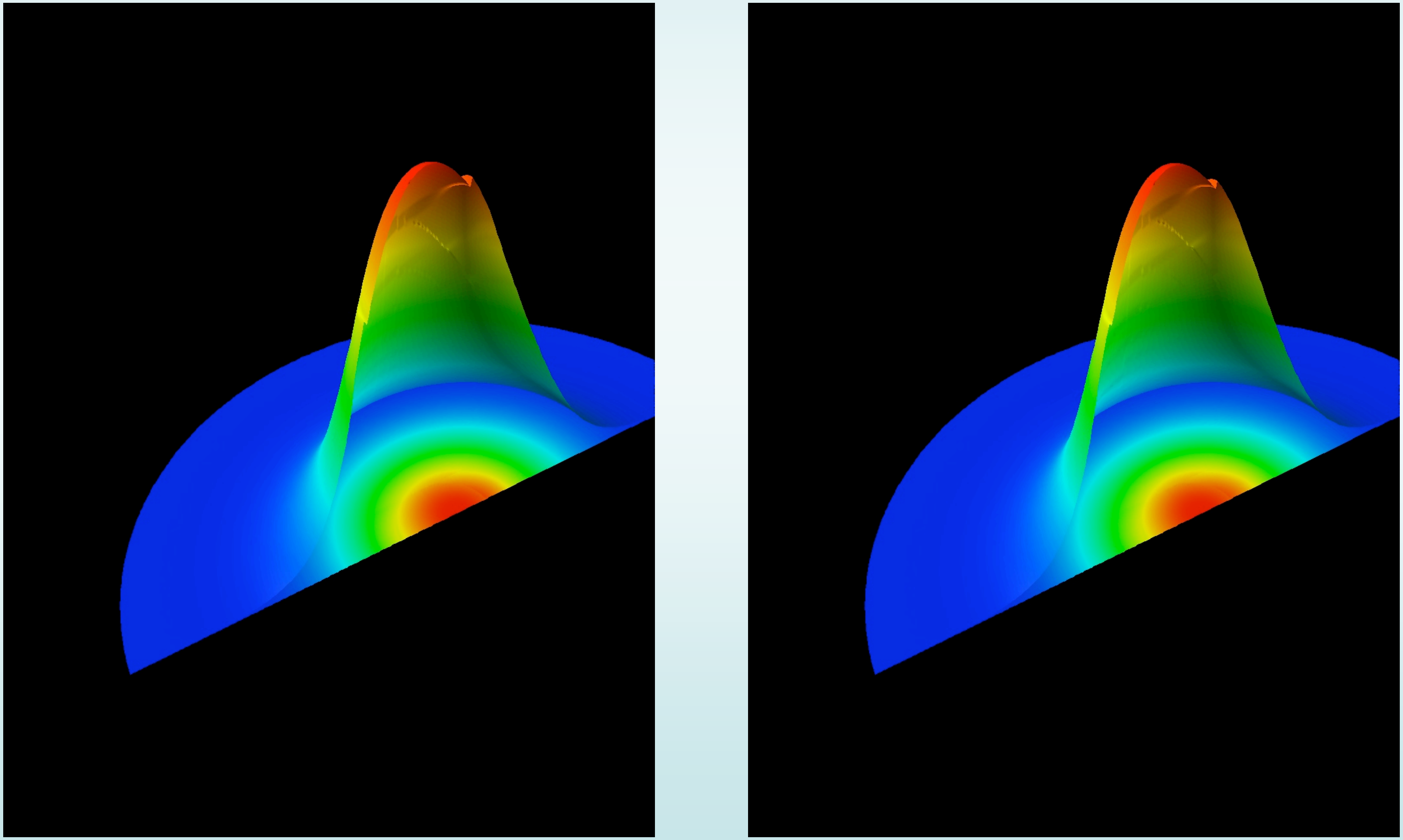




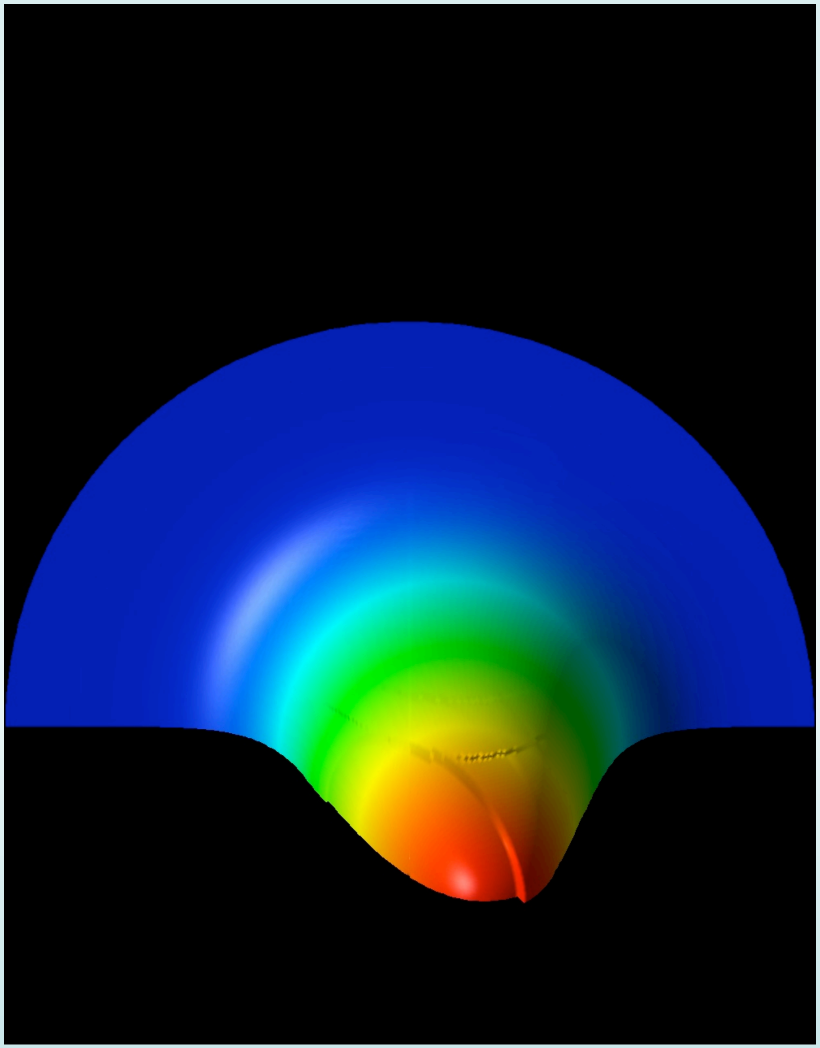
Drifting Maxwellian Test
Non-Linear Self Collision Annihilation

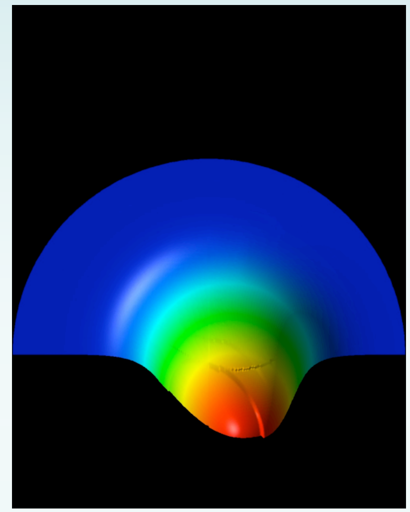
$t = 0 : n = .99813, u = .099847, E = 1.51792$

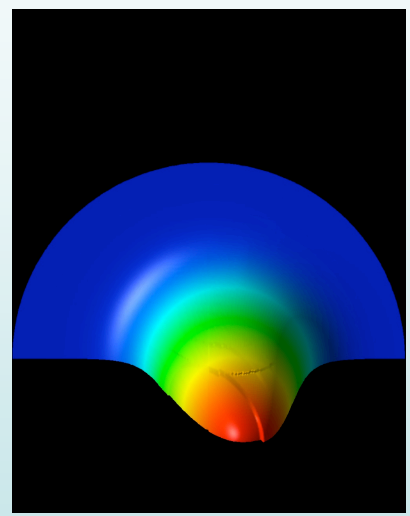
$t = 3\tau_{ii} : n = .99813, u = .100249, E = 1.51564$



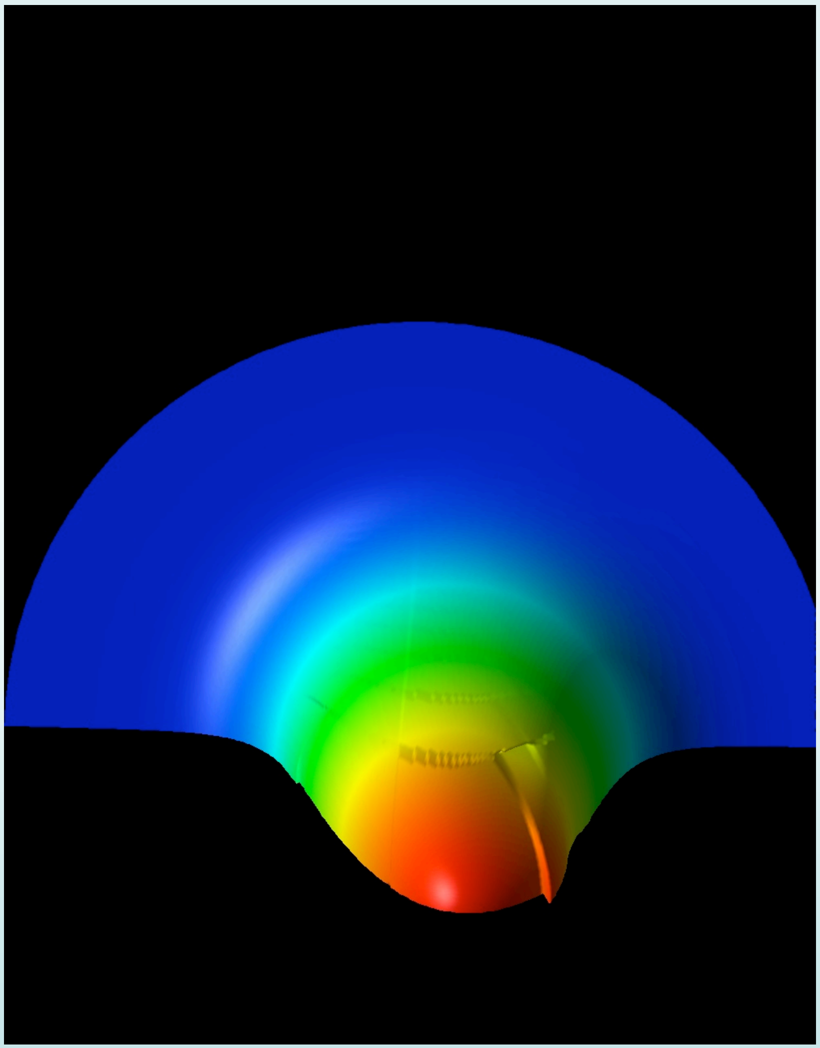
Minimum B Reconstruction stable





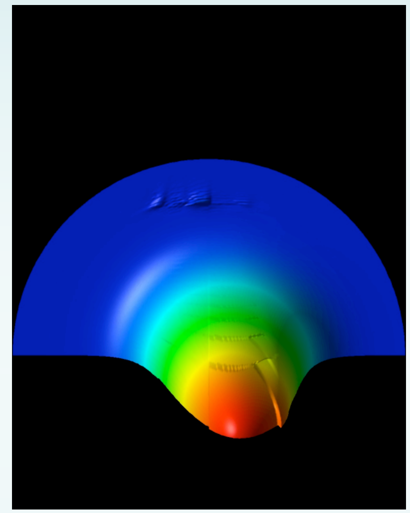


Maximum B Reconstruction can exhibit feedback instability

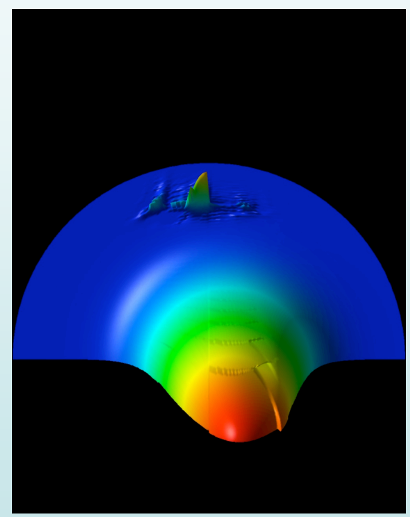


n=0

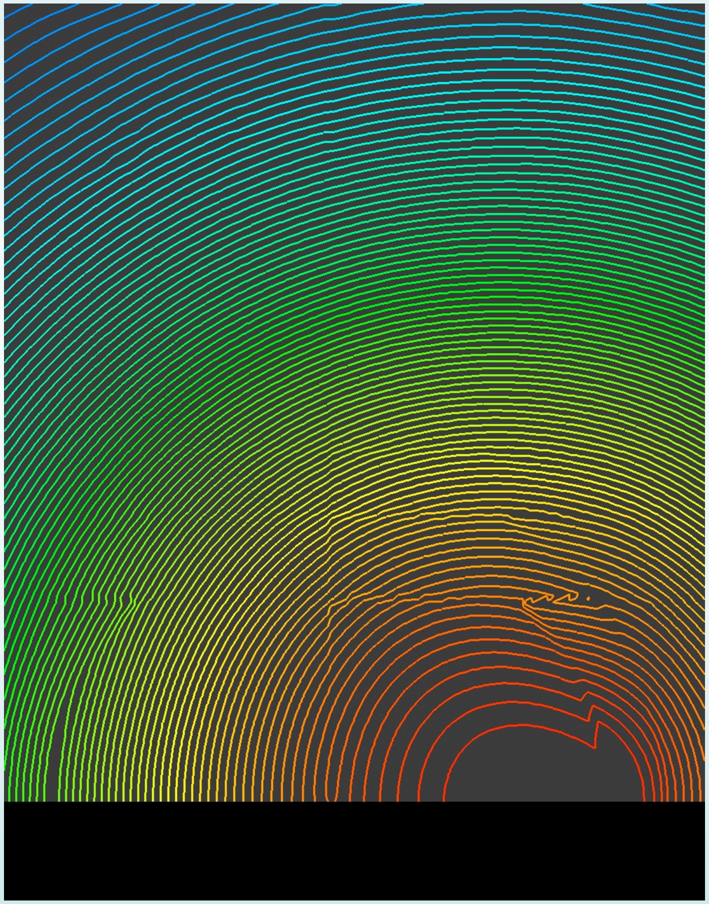
n=100

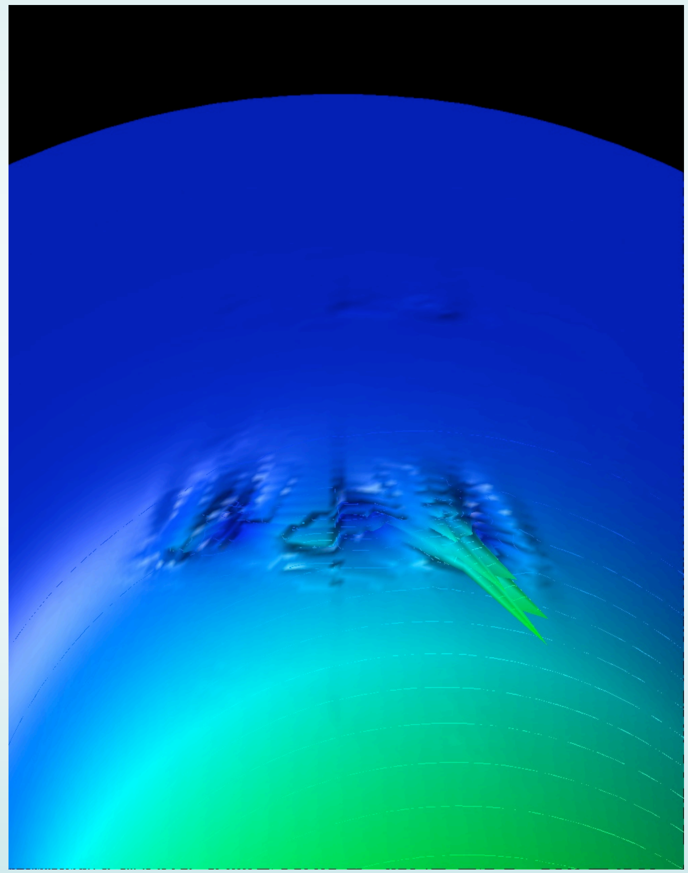


n=200



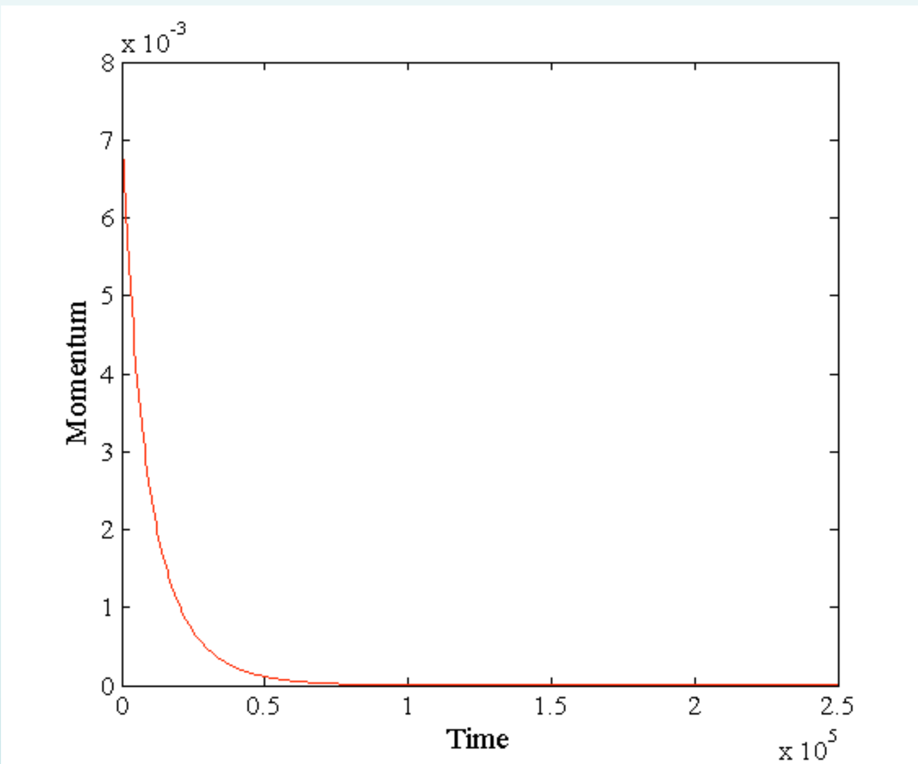
Algorithmic instability begins at particle turning points, at high E, and at high B/B0

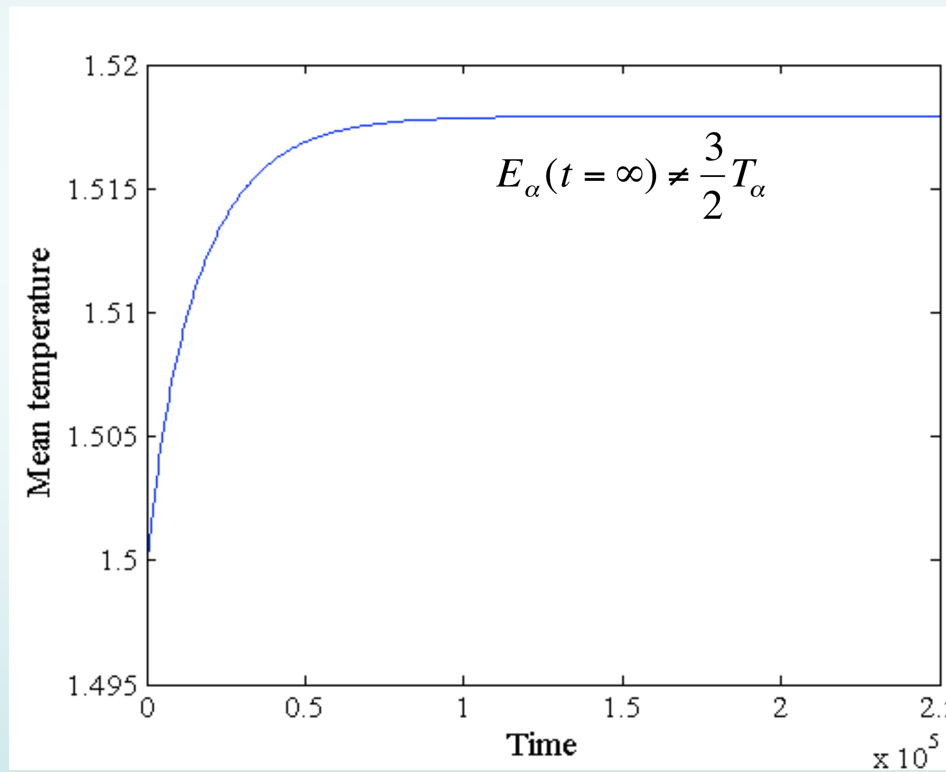




Non-Maxwellian I.C

- The initial non-zero mean momentum of the test particles decays to zero through the collision with the field particles.
- But, since the FPC is linear, the test particles do not relax into a Maxwellian! Only a nonlinear FPC, accounting for the particle's self-collision, can lead that.





Summary

- We have formulated and implemented a nonlinear Fokker-Planck collision operator in constants-of-motion velocity coordinates, namely, the energy E and magnetic moment μ.
- The turning point boundary ($v_{||}=0$) in (E, μ) space is carefully treated with a cut cell algorithm. The resulting cells (both cut and uncut) are then mapped directly into ($v_{||}$, μ) space for numerical implementation. This obviates the need of numerical interpolation between coordinates, which is typically inaccurate and non-conservative.
- In ($v_{||}$, μ) space, a high order finite volume approach is developed to ensure complete particle conservation. A linear collision operator based on this methodology has been applied to the problems of thermal equilibration, and the computation results show quantitative agreement with theory.
- A fully nonlinear operator has been developed for TEMPEST based on a this approach using the Rosenbluth potentials computed in an adaptation of FPPAC (CQL) and the 4^{th} order cutcell reconstruction algorithm. Early results show excellent momentum conservation for selectively chosen meshes.
- Stay tuned.